



chain nodes :

13 14 15 16 17 19 22 23 24 25 26 27 39 40 41 42 53 60 61

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 43 44 45 54 55 56 57 58 59

chain bonds :

3-61 4-7 5-39 6-60 13-14 13-15 16-17 17-19 22-23 23-24 25-26 26-27 39-53 40-41  
40-42 53-55

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 43-44 43-45 44-45  
54-55 54-59 55-56 56-57 57-58 58-59

exact/norm bonds :

5-39 13-14 13-15 17-19 22-23 23-24 39-53 43-44 43-45 44-45 53-55

exact bonds :

3-61 4-7 6-60 16-17 25-26 26-27 40-41 40-42

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 54-55 54-59 55-56  
56-57 57-58 58-59

isolated ring systems :

containing 1 :

G1:O,N

G2:[\*1-\*2],[\*3-\*4],[\*5-\*6],[\*7-\*8]

G3:CH2,[\*9-\*10],[\*11-\*12]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:Atom  
44:Atom 45:Atom 53:CLASS 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:CLASS  
61:CLASS